

Diphenylamine
122-39-4 | DTXSID4021975

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 4.17e-03 mol/L

Global applicability domain: Inside

Local applicability domain index: 4.86e-01

Confidence level: 4.47e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Heptachlor epoxide</div> <div>Measured: 5.14e-07</div> <div>Predicted: 3.52e-07</div>	<div>Image not found</div> <div>2-Mercaptobenzoxazole</div> <div>Measured: 6.61e-03</div> <div>Predicted: 5.97e-02</div>	<div>Image not found</div> <div>N-(1-Naphthyl)ethylenediamine</div> <div>Measured: 1.07e-02</div> <div>Predicted: 9.11e-02</div>
<div>Image not found</div> <div>Quinoxaline</div> <div>Measured: 5.07</div> <div>Predicted: 1.30e-01</div>	<div>Image not found</div> <div>1,10-Phenanthroline</div> <div>Measured: 1.49e-02</div> <div>Predicted: 5.60e-03</div>	